

Steady State Global Simulations of Microturbulence

W. W. Lee

Princeton Plasma Physics Laboratory
(November 2004)

In collaboration with

S. Ethier, S. Klasky, J. L. V. Lewandowski, W. X. Wang, G. Rewoldt
and T. S. Hahm (PPPL)
Y. Nishimura, and Z. Lin (UC-Irvine)

Supported by

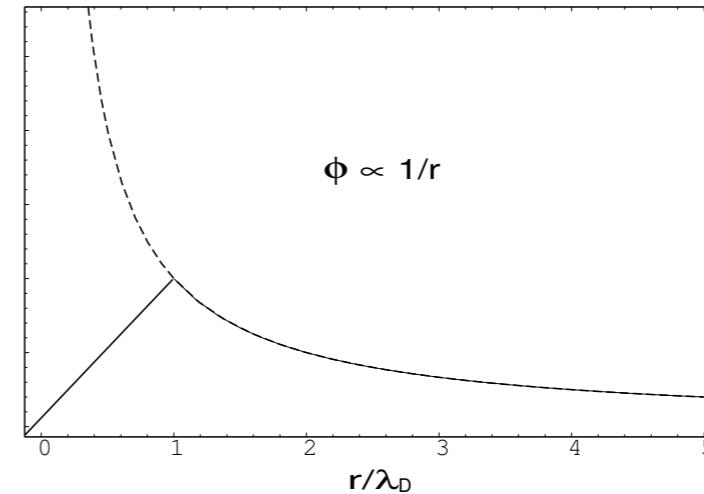
DoE SciDAC Center for Gyrokinetic Particle Simulation
of Turbulent Transport in Burning Plasmas

Outline

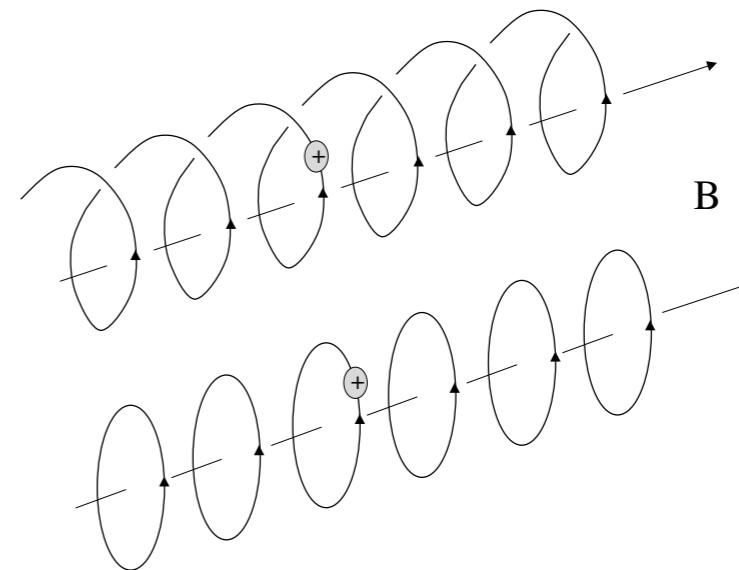
- Basics of Gyrokinetic Particle Simulation
 - Finite size particles
 - Decoupling of gyromotion and polarization effects
 - Governing equations
- Gyrokinetic Particle Simulation of Microturbulence
 - Simulation using the Gyrokinetic Toroidal Code (GTC)
 - Scalability on MPP machines
 - Influence of Parallel Velocity-Space Nonlinearity on Steady State Microturbulence
- Integrated Plasma Simulation
 - Core-Edge Simulations
 - Transport Time Scale Simulations

Basics of Gyrokinetic Particle Simulation

- Finite-size particles
[Dawson et al. '68; Birdsall et al. '68]
 - Coulomb interactions are collisionless
 - Collisional effects are subgrid phenomena



- Gyrokinetic particles
[Lee PF '83]
 - Gyromotion becomes motion of rotating charged rings
 - Polarization Effects in the field equations



- Efficient numerical methods to account for finite Larmor radius effects
[Lee JCP '87; Lee and Qin PP '03]

Gyrokinetic Vlasov-Maxwell Equations in Toroidal Geometry

- GK Vlasov equation - in gyrocenter coordinates

[Lee PF '83; Hahm et al. PF '88; Hahm PF '88; Brizard PF '88; Brizard J. Plas. Phys. '89; Qin et al. PoP '99; Qin et al. PoP '00; Qin et al., PoP '00; Lee and Qin PoP '03]

$$\frac{\partial F_{\alpha gc}}{\partial t} + \frac{d\mathbf{R}}{dt} \cdot \frac{\partial F_{\alpha gc}}{\partial \mathbf{R}} + \frac{dv_{\parallel}}{dt} \frac{\partial F_{\alpha gc}}{\partial v_{\parallel}} = 0,$$

$$\frac{d\mathbf{R}}{dt} = v_{\parallel} \mathbf{b}^* + \frac{v_{\perp}^2}{2\Omega_{\alpha 0}} \hat{\mathbf{b}}_0 \times \nabla \ln B_0 - \frac{c}{B_0} \nabla \bar{\phi} \times \hat{\mathbf{b}}_0$$

$$\frac{dv_{\parallel}}{dt} = -\frac{v_{\perp}^2}{2} \mathbf{b}^* \cdot \nabla \ln B_0 - \boxed{\frac{q_{\alpha}}{m_{\alpha}} \left(\mathbf{b}^* \cdot \nabla \bar{\phi} + \frac{1}{c} \frac{\partial \bar{A}_{\parallel}}{\partial t} \right)} \quad \text{-- Velocity Nonlinearity}$$

$$\mu_B \equiv \frac{v_{\perp}^2}{2B_0} \left(1 - \frac{mc}{e} \frac{v_{\parallel}}{B_0} \hat{\mathbf{b}}_0 \cdot \nabla \times \hat{\mathbf{b}}_0 \right) \approx \text{cons.}$$

$$\mathbf{b}^* \equiv \mathbf{b} + \frac{v_{\parallel}}{\Omega_{\alpha 0}} \hat{\mathbf{b}}_0 \times (\hat{\mathbf{b}}_0 \cdot \nabla) \hat{\mathbf{b}}_0, \quad \mathbf{b} = \hat{\mathbf{b}}_0 + \frac{\nabla \times \bar{\mathbf{A}}}{B_0}$$

$$\begin{pmatrix} \bar{\phi} \\ \bar{\mathbf{A}} \end{pmatrix}(\mathbf{R}) = \langle \int \begin{pmatrix} \phi \\ \mathbf{A} \end{pmatrix}(\mathbf{x}) \boxed{\delta(\mathbf{x} - \mathbf{R} - \rho)} d\mathbf{x} \rangle_{\varphi}, \quad \text{-- Coordinate Transformation}$$

$$F_{\alpha gc} = \sum_{j=1}^{N_{\alpha}} \delta(\mathbf{R} - \mathbf{R}_{\alpha j}) \delta(\mu - \mu_{\alpha j}) \delta(v_{\parallel} - v_{\parallel \alpha j})$$

GK Equations in Toroidal Geometry (cont.)

- GK Poisson's equation - in laboratory coordinates [Lee JCP '87]

$$\nabla^2 \phi + \frac{\tau}{\lambda_D^2} [\phi(\mathbf{x}) - \tilde{\phi}(\mathbf{x})] = -4\pi \rho_{gc}(\mathbf{x}) \quad \xrightarrow{(k_\perp \rho_i)^2 \ll 1} \quad \boxed{\frac{\rho_s^2}{\lambda_D^2} \nabla_\perp^2 \phi(\mathbf{x}) = -4\pi \rho_{gc}(\mathbf{x})}$$

$$\tilde{\phi}(\mathbf{x}) \equiv \langle \int \bar{\phi}(\mathbf{R}) F_i(\mathbf{R}, \mu, v_\parallel) \delta(\mathbf{R} - \mathbf{x} + \rho) d\mathbf{R} d\mu dv_\parallel \rangle_\varphi$$

$$\rho_{gc}(\mathbf{x}) = \sum_\alpha q_\alpha \langle \int F_{\alpha gc}(\mathbf{R}) \delta(\mathbf{R} - \mathbf{x} + \rho) d\mathbf{R} dv_\parallel d\mu \rangle_\varphi$$

- GK Ampere's law -- in laboratory coordinates [Qin et al. PP '99]

$$\boxed{\nabla^2 \mathbf{A} - \frac{1}{v_A^2} \cancel{\frac{\partial^2 \mathbf{A}_\perp}{\partial t^2}} = -\frac{4\pi}{c} \mathbf{J}_{gc}} \quad \omega^2/k^2 v_A^2 \ll 1$$

$$\mathbf{J}_{gc}(\mathbf{x}) = \mathbf{J}_{\parallel gc}(\mathbf{x}) + \mathbf{J}_{\perp gc}^M(\mathbf{x}) + \mathbf{J}_{\perp gc}^d(\mathbf{x})$$

$$= \sum_\alpha q_\alpha \langle \int (\mathbf{v}_\parallel + \mathbf{v}_\perp + \mathbf{v}_d) F_{\alpha gc}(\mathbf{R}) \delta(\mathbf{R} - \mathbf{x} + \rho) d\mathbf{R} dv_\parallel d\mu \rangle_\varphi$$

$$\mathbf{v}_d \equiv \frac{v_\parallel^2}{\Omega_{\alpha 0}} \hat{\mathbf{b}}_0 \times (\hat{\mathbf{b}}_0 \cdot \nabla) \hat{\mathbf{b}}_0 + \frac{v_\perp^2}{2\Omega_{\alpha 0}} \hat{\mathbf{b}}_0 \times \nabla \ln B_0$$

GK Equations in Toroidal Geometry (cont.)

- Calculations of FLR effects for $k_{\perp} \rho_i \sim 1$ is only possible in the gyrocenter coordinates, but not in the laboratory coordinates

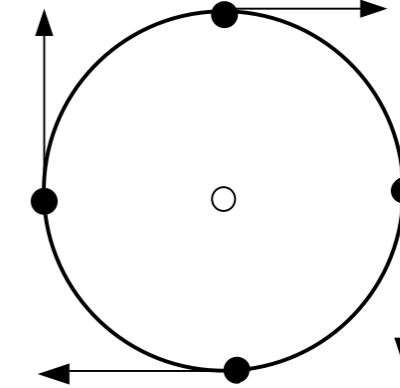
$$\begin{pmatrix} \bar{\phi} \\ \bar{\mathbf{A}} \end{pmatrix}(\mathbf{R}_{\alpha j}) = \langle \begin{pmatrix} \phi \\ \mathbf{A} \end{pmatrix}(\mathbf{x}_{\alpha j}) \rangle_{\varphi}$$

$$\rho_{gc}(\mathbf{x}) = \sum_{\alpha} q_{\alpha} \sum_{j=1}^N \langle \delta(\mathbf{x} - \mathbf{x}_{\alpha j}) \rangle_{\varphi}$$

$$\mathbf{J}_{\parallel gc}(\mathbf{x}) = \sum_{\alpha} q_{\alpha} \sum_{j=1}^N v_{\parallel \alpha j} \langle \delta(\mathbf{x} - \mathbf{x}_{\alpha j}) \rangle_{\varphi}$$

$$\mathbf{J}_{\perp gc}^M(\mathbf{x}) = \sum_{\alpha} q_{\alpha} \sum_{j=1}^N \langle \mathbf{v}_{\perp \alpha j} \delta(\mathbf{x} - \mathbf{x}_{\alpha j}) \rangle_{\varphi}$$

$$\mathbf{J}_{\perp gc}^d(\mathbf{x}) = \sum_{\alpha} q_{\alpha} \sum_{j=1}^N \langle \mathbf{v}_{d\alpha j} \delta(\mathbf{x} - \mathbf{x}_{\alpha j}) \rangle_{\varphi}$$



Coordinate Transformation

- Perpendicular current for $k_{\perp} \rho_i \ll 1$ [Qin et al. PP '00]

$$\mathbf{J}_{\perp gc} = \mathbf{J}_{\perp gc}^M + \mathbf{J}_{\perp gc}^d = \frac{c}{B_0} \sum_{\alpha} \left[\hat{\mathbf{b}}_0 \times \nabla p_{\alpha \perp} + (p_{\alpha \parallel} - p_{\alpha \perp})(\nabla \times \hat{\mathbf{b}}_0)_{\perp} \right]$$

- Pressure Balance: $p = p_{\alpha \parallel} = p_{\alpha \perp}$

$$\mathbf{J}_{\perp gc} = \frac{c}{B_0} \sum_{\alpha} \hat{\mathbf{b}}_0 \times \nabla p_{\alpha}$$

Reduced MHD Equations vs. Gyrokinetic-MHD Equations⁷

- GK Three-field Equations for $k_{\perp} \rho_i \ll 1$ w/o geometric simplification [Lee and Qin PP '03]

$$\frac{d}{dt} \nabla_{\perp}^2 \phi + \frac{v_A^2}{c} (\hat{\mathbf{b}} \cdot \nabla) \nabla^2 A_{\parallel} - \boxed{4\pi \frac{v_A^2}{c^2} \nabla_{\perp} \cdot \mathbf{J}_{\perp gc}^d} = 0$$

$$\frac{1}{c} \frac{\partial A_{\parallel}}{\partial t} + \mathbf{b} \cdot \nabla \phi = 0.$$

$$\frac{dp_{\alpha}}{dt} = 0$$

$$\frac{d}{dt} \equiv \frac{\partial}{\partial t} - \frac{c}{B} \nabla \bar{\phi} \times \hat{\mathbf{b}}_0 \cdot \nabla$$

$$\mathbf{J}_{\perp gc}^d = \frac{c}{B_0} \sum_{\alpha} \left[p_{\alpha} (\nabla \times \hat{\mathbf{b}}_0)_{\perp} + p_{\alpha} \hat{\mathbf{b}}_0 \times (\nabla \ln B_0) \right]$$

- Reduced High- β Three-Field MHD Equations [Strauss PF '78]

$$\frac{d \nabla_{\perp}^2 \phi}{dt} + \frac{v_A^2}{c} (\hat{\mathbf{b}} \cdot \nabla) \nabla_{\perp}^2 A_{\parallel} - \boxed{\frac{2}{R_0} \frac{\partial p}{\partial y}} = 0$$

$$\frac{1}{c} \frac{\partial A_{\parallel}}{\partial t} + \mathbf{b} \cdot \nabla \phi = 0.$$

$$\frac{dp}{dt} = 0$$

Magnetic Field Calculations

- For given zeroth-order field and density, parallel current and temperature profiles

$$\mathbf{J}_{\parallel gc}(\mathbf{x}) = \sum_{\alpha} q_{\alpha} \sum_{j=1}^N v_{\parallel \alpha j} \langle \delta(\mathbf{x} - \mathbf{x}_{\alpha j}) \rangle_{\varphi}$$

$$\mathbf{J}_{\perp gc}^M(\mathbf{x}) = \sum_{\alpha} q_{\alpha} \sum_{j=1}^N \langle \mathbf{v}_{\perp \alpha j} \delta(\mathbf{x} - \mathbf{x}_{\alpha j}) \rangle_{\varphi}$$

$$\mathbf{J}_{\perp gc}^d(\mathbf{x}) = \sum_{\alpha} q_{\alpha} \sum_{j=1}^N \mathbf{v}_{d\alpha j} \langle \delta(\mathbf{x} - \mathbf{x}_{\alpha j}) \rangle_{\varphi}$$

- Ampere's law

$$\nabla^2 \mathbf{A} = -\frac{4\pi}{c} \mathbf{J}_{gc}$$

$$\mathbf{B} = \nabla \times \mathbf{A}$$

- FLR effects are taken into account in gyrocenter space

Fluctuation-Dissipation Theorem and Particle Simulation

- Plasma Waves and Finite-Size Particles [Langdon and Birdsall, PF 13, 2115 (1970)]

$$V \frac{|\mathbf{E}(\mathbf{k})|^2}{8\pi} = \frac{T/2}{1 + k^2 \lambda_D^2 / S^2} \rightarrow T/2, \quad V \text{-- volume, } S \text{ -- particle shape}$$

- Gyrokinetic Particle Simulation [Krommes et al., PF '86; Lee, JCP '87]

$$V \frac{|\mathbf{E}(\mathbf{k})|^2}{8\pi} = \frac{\lambda_D^2}{\rho_s^2} (T/2) \quad \text{for} \quad k\rho_i \ll 1$$

- Shear-Alfven Waves in Gyrokinetic Plasmas [Lee et al., PP '01]

$$V \frac{|\mathbf{E}(\mathbf{k})|^2}{8\pi} = \frac{\lambda_D^2}{\rho_s^2} \frac{T/2}{1 + \omega_{pe}^2/c^2 k^2}, \quad \text{cold electrons}$$

$$V \frac{|\mathbf{E}(\mathbf{k})|^2}{8\pi} = k^2 \lambda_D^2 \frac{T/2}{1 + k^2 \rho_s^2}, \quad \text{warm electrons}$$

- Compressional-Alfven Waves in Gyrokinetic Plasmas

$$\frac{A_\perp}{A_\parallel} \sim \frac{\omega^2}{k^2 v_A^2} \ll 1$$

Perturbative Particle Simulation

- δf simulation schemes:

-- [Dimits and Lee, JCP '93; Parker and Lee, PF '93]

$$\text{Let } F = F_0 + \delta f \longrightarrow \frac{d\delta f}{dt} = -\frac{dF_0}{dt}$$

$$\text{Let } w \equiv \frac{\delta f}{F} \longrightarrow \delta f = \sum_{j=1}^N w_j \delta(\mathbf{R} - \mathbf{R}_j) \delta(\mu - \mu_j) \delta(v_{\parallel} - v_{\parallel j})$$

Noise reduction: $|E|^2 \propto w^2$ [Hu and Krommes, PoP '94]

-- [Aydemir, PoP '94]

$$F = F_0 + \delta f \longrightarrow w \equiv \frac{\delta n}{n}$$

- Split-weight schemes: [Manuilskiy and Lee, PoP '00; Lee et al., PoP '01, Lewnadowski, PoP '03]

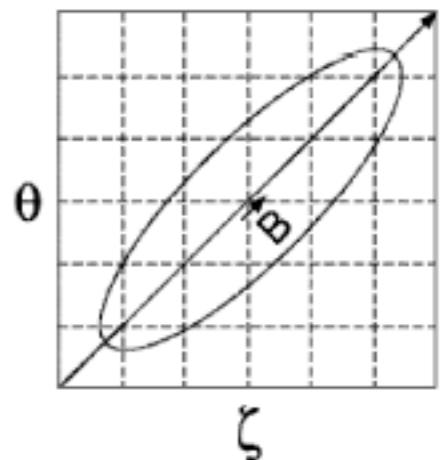
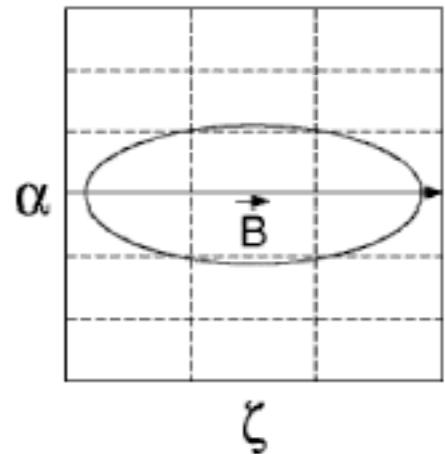
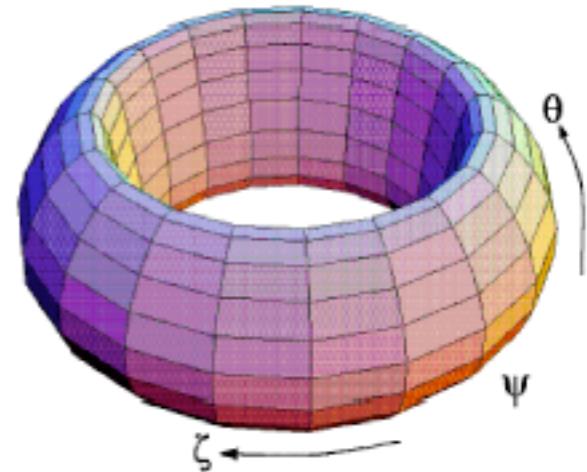
$$F = F_0 + \psi F_0 + \delta h \quad \psi = \phi + \frac{1}{c} \int \frac{\partial A_{\parallel}}{\partial t} dx_{\parallel 0}$$

- Hybrid Scheme [Lin and Chen, PoP '01]
- Time step is determined by zeroth order transit time of the electrons along the field line.

Global Gyrokinetic Toroidal Particle Simulation Code: GTC

[Z. Lin, T. S. Hahm, W. W. Lee, W. M. Tang and R. B. White, *Science* (1998)]

- Magnetic coordinates (ψ, θ, ζ) [Boozer, 1981]
- Guiding center Hamiltonian [Boozer, 1982; White and Chance, 1984]
- Non-spectral Poisson solver [Lin and Lee, 1995]
- Global field-line coordinates: (ψ, α, ζ) , $\alpha = \theta - \zeta/q$
 - Microinstability wavelength: $\lambda_{\perp} \propto \rho_i$, $\lambda_{\parallel} \propto qR$
 - With field-line coordinates: Grid # $N \propto a^2$, a : minor radius, $\Delta\zeta \propto R$
 - Without field-line coordinates: grid # $N \propto a^3$, $\Delta\zeta \propto \rho$
 - Larger time step: no high k_{\parallel} modes
- Collisions: e-i, i-i and e-e
- Neoclassical Transport Code: GTC-neo [W. X. Wang, 2004]



Global Turbulence Code (GTC)



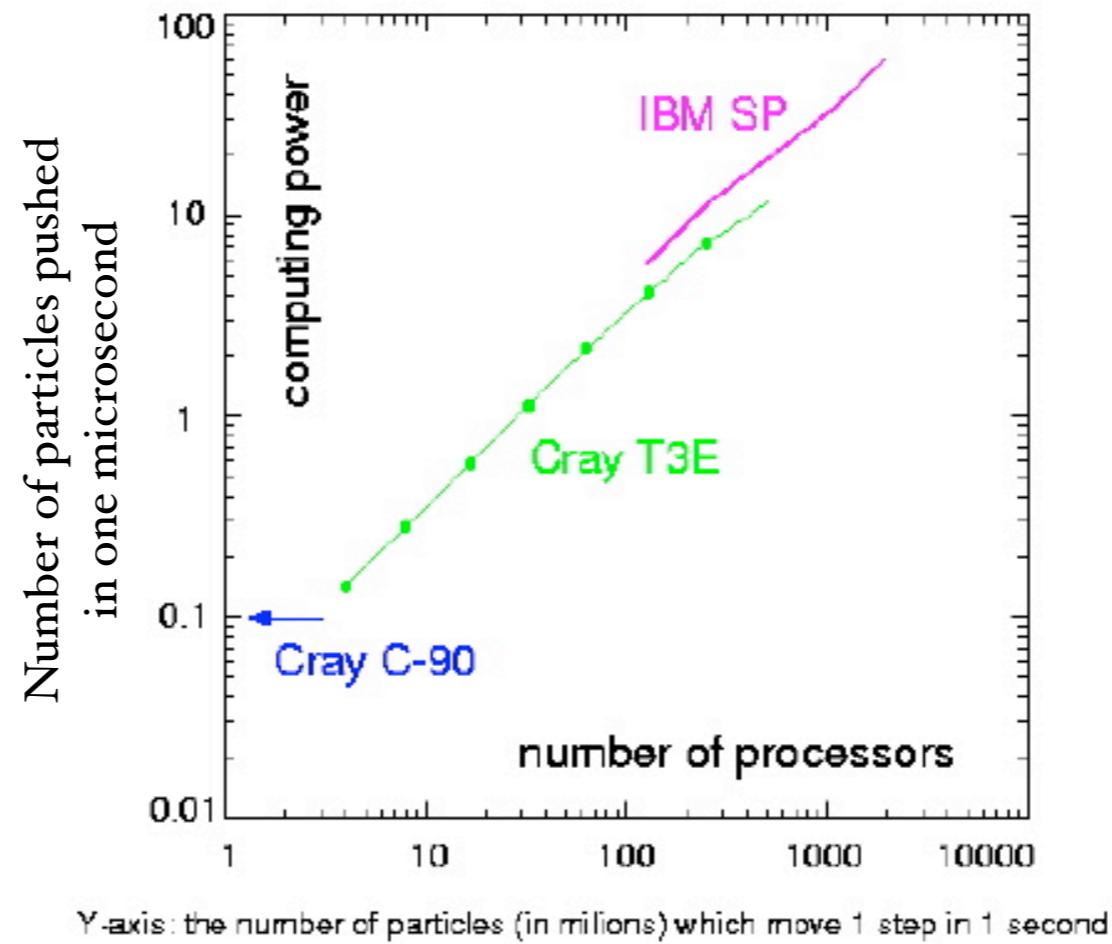
Single Processor Performance (S. Ethier)

Processor	Max speed (Mflops)	GTC test (Mflops)	Efficiency (real/max)	Relative speed (user time)
Power3 (Seaborg)	1,500	173.6	12 %	1
Power4 (Cheetah)	5,200	304.5	6 %	1.9
SX6 (Rime)	8,000	715.7	9 %	5.2

Earth Simulator 25% 10 (Ethier)
 3.7 TeraFlop with 2048 processors using 5 billion particles



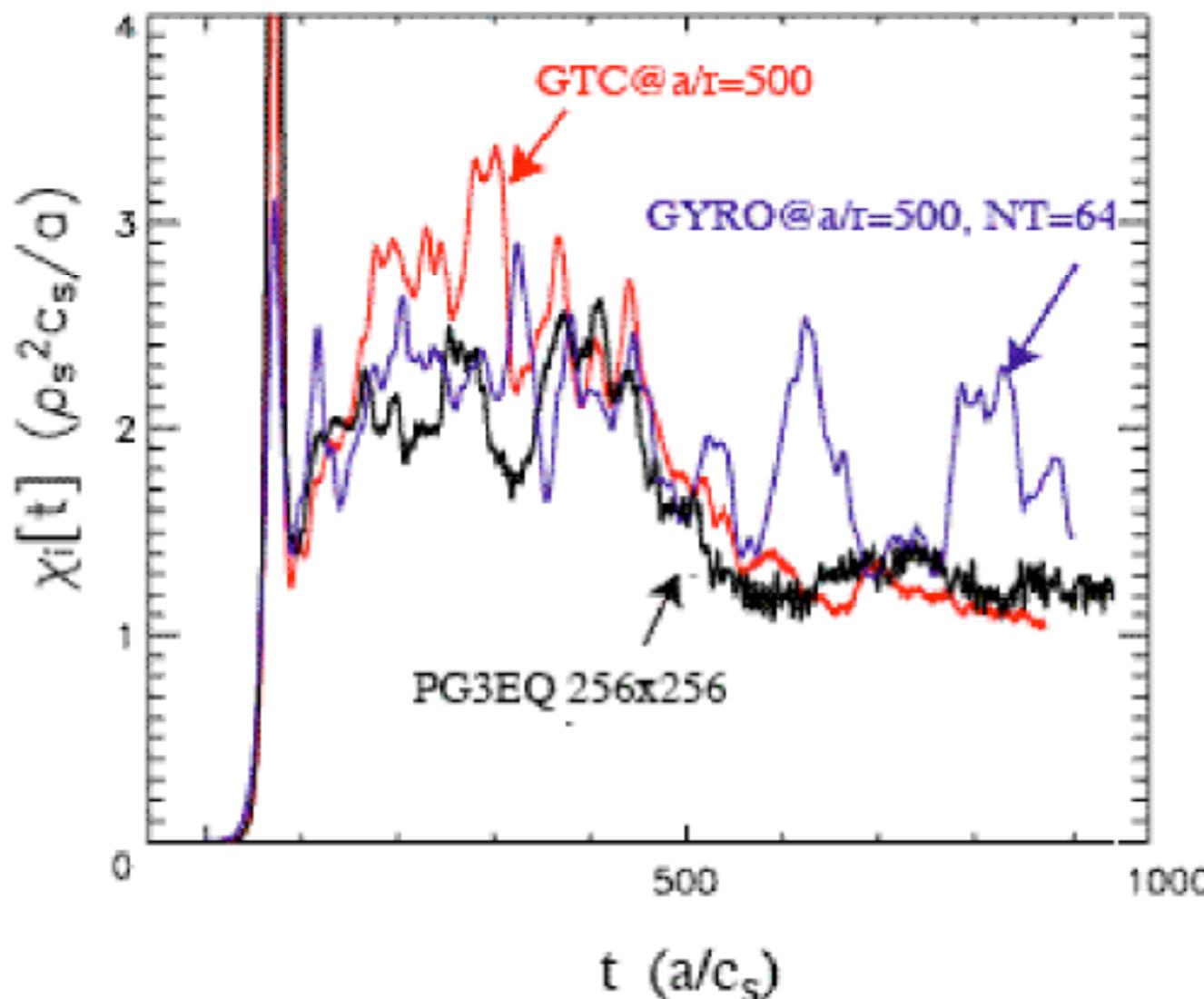
GTC Scalable to a Large Number of processors (Lin and Ethier)



GTC size scaling studies (Lin et al. 2002 IAEA): 1 billion particles (8 particles/cell) for $a/\rho_s = 1000$ using 1024 processors on IBM-SP for 7000 time-steps took 72 wallclock hours to simulate 1 msec of discharge.

Recent PMP Code Comparisons and Controversies

(W. M. Nevins, 04)

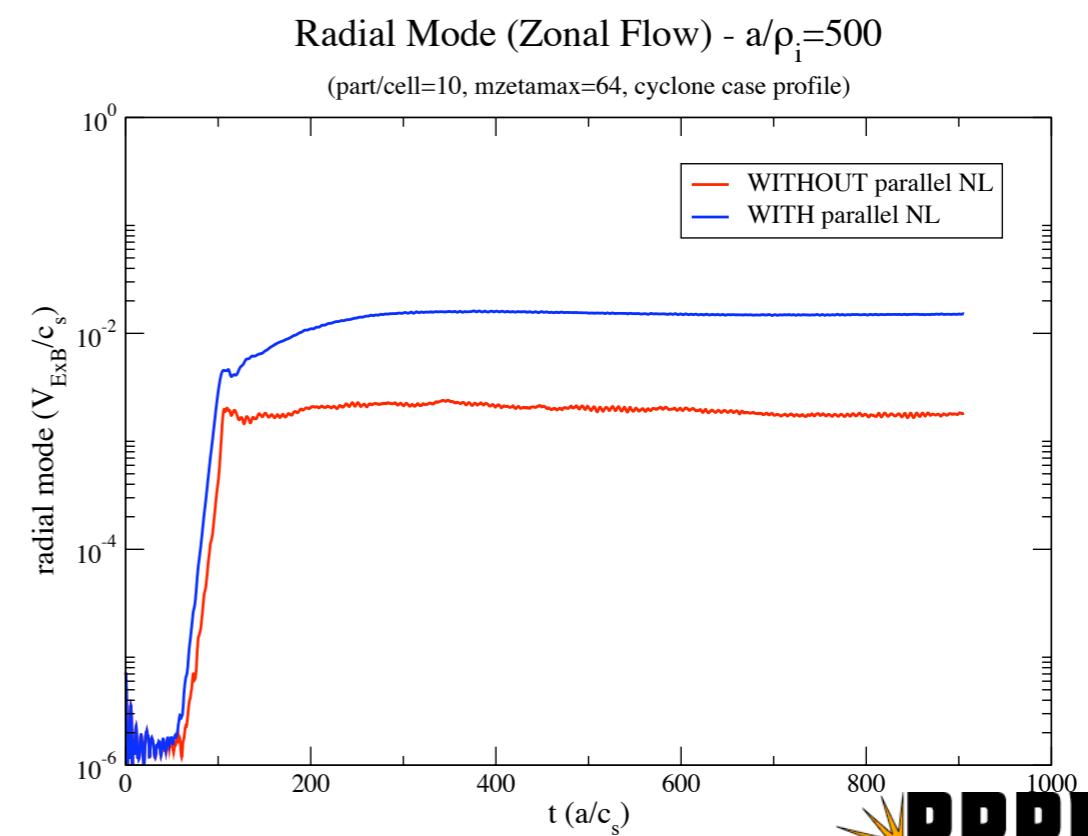
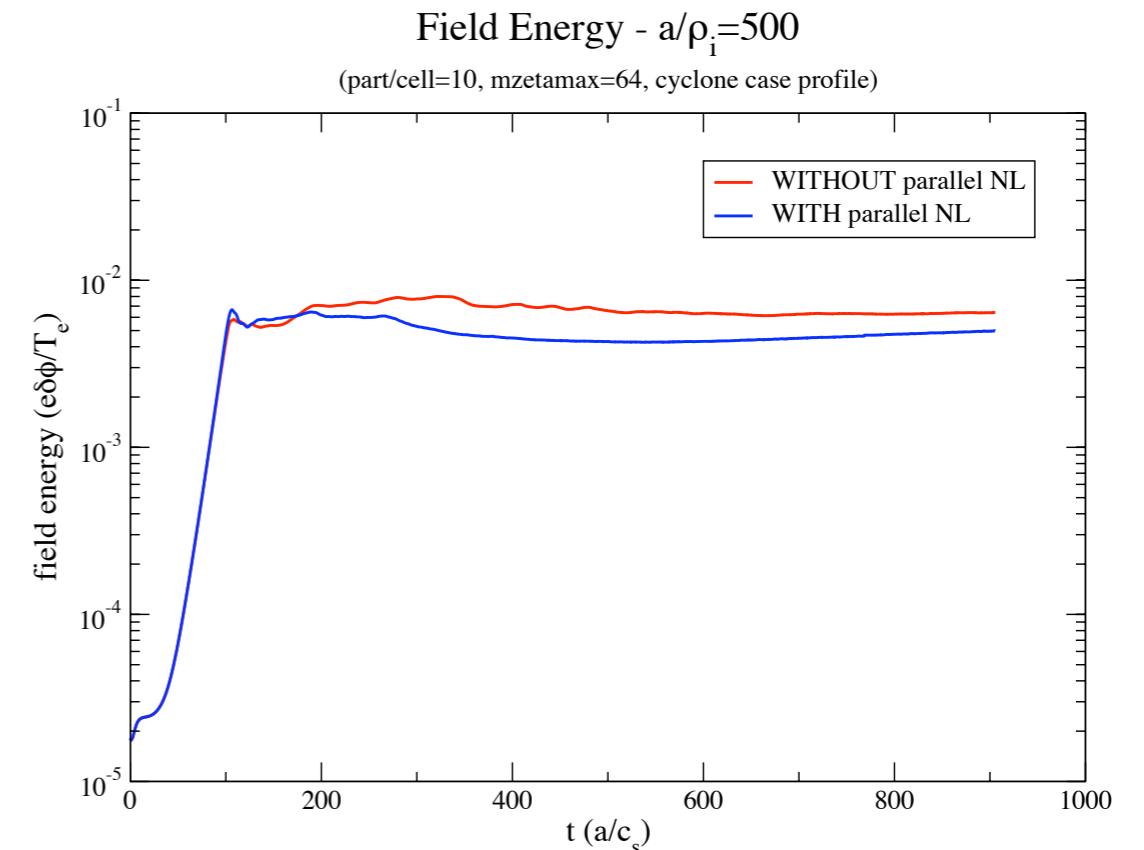
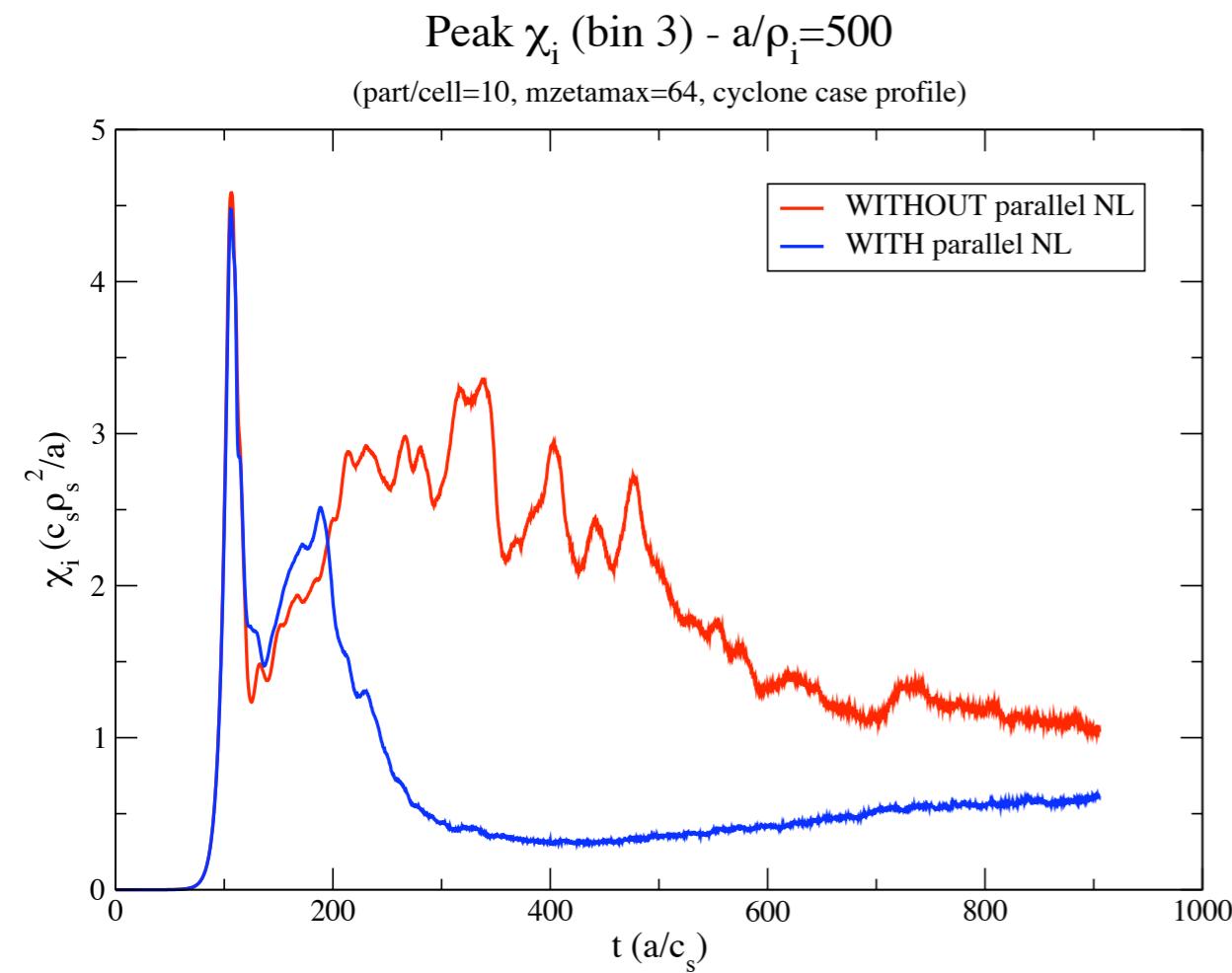


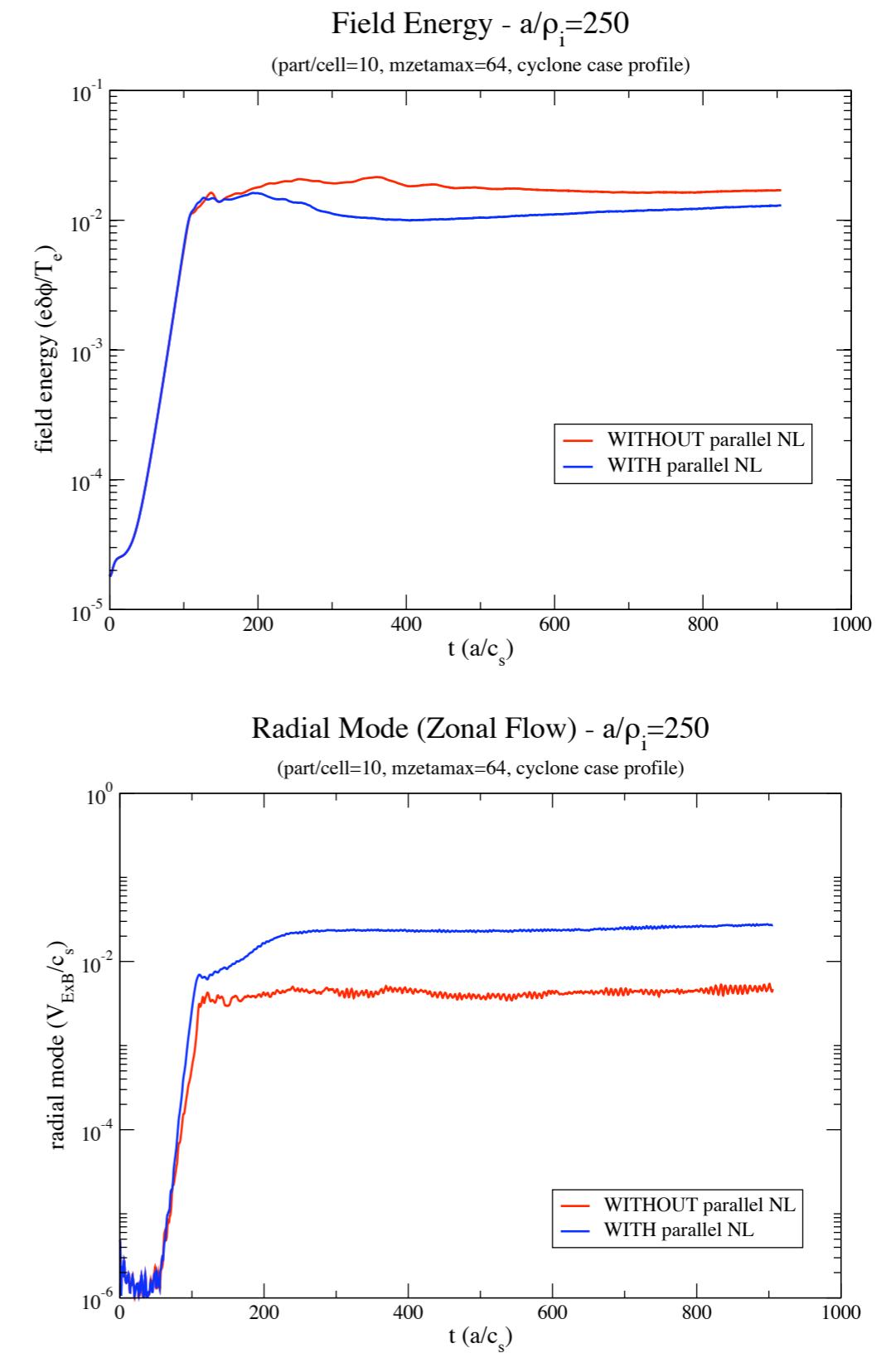
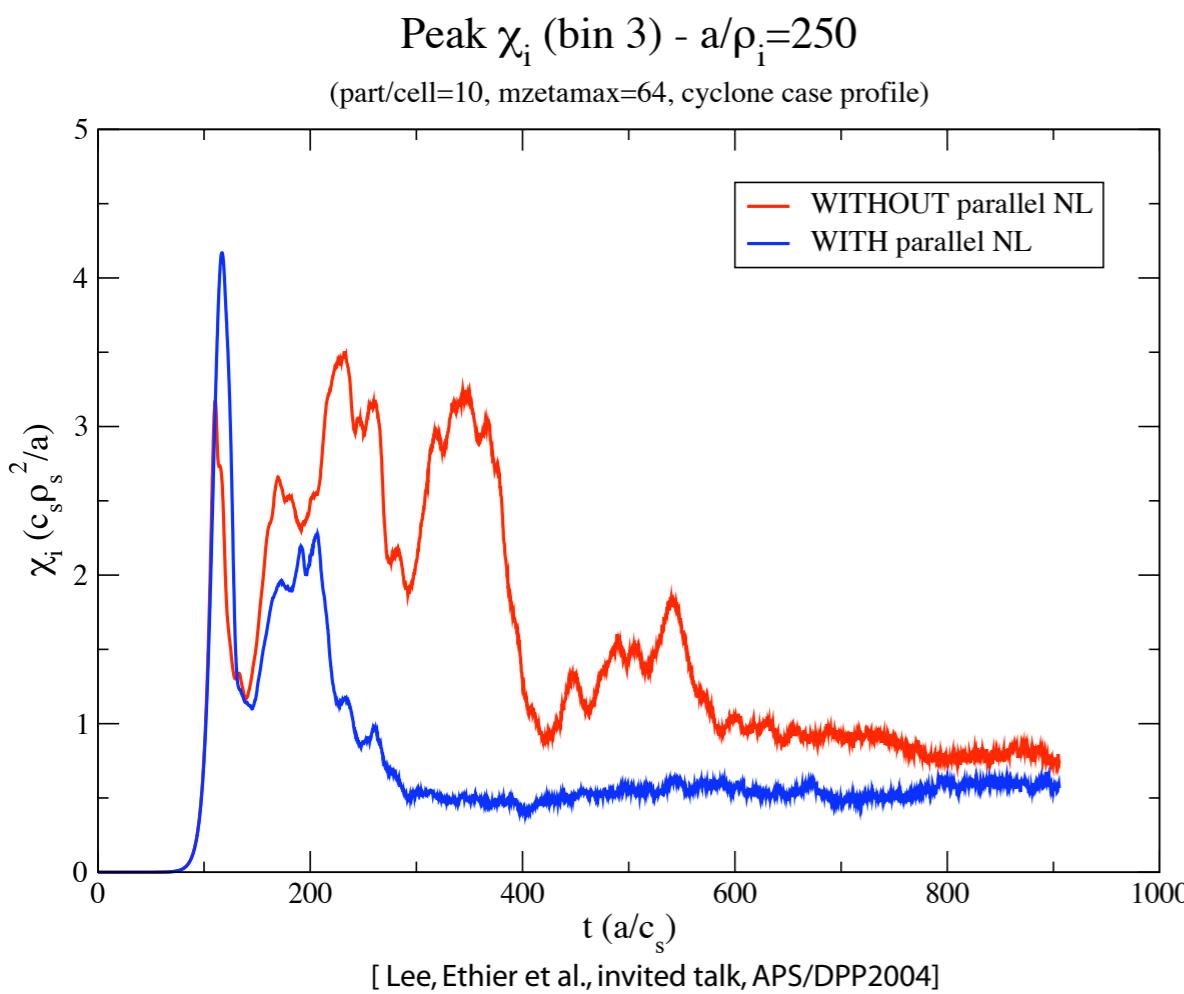
Code Comparisons:

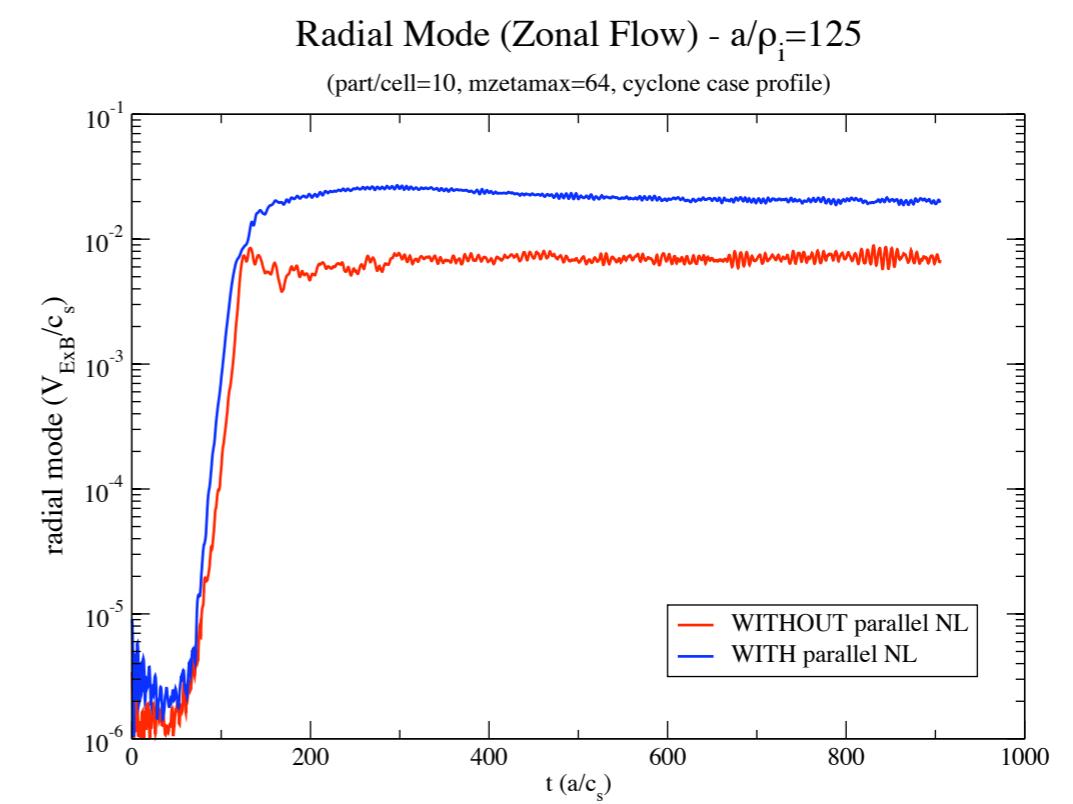
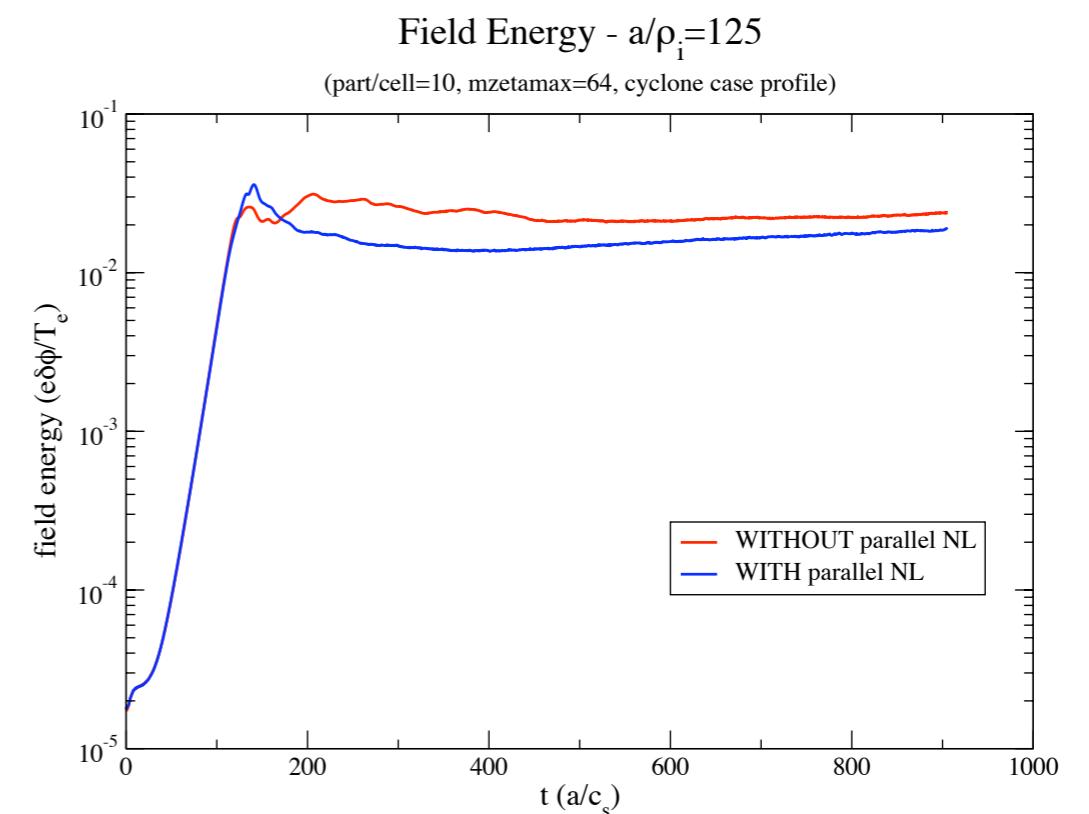
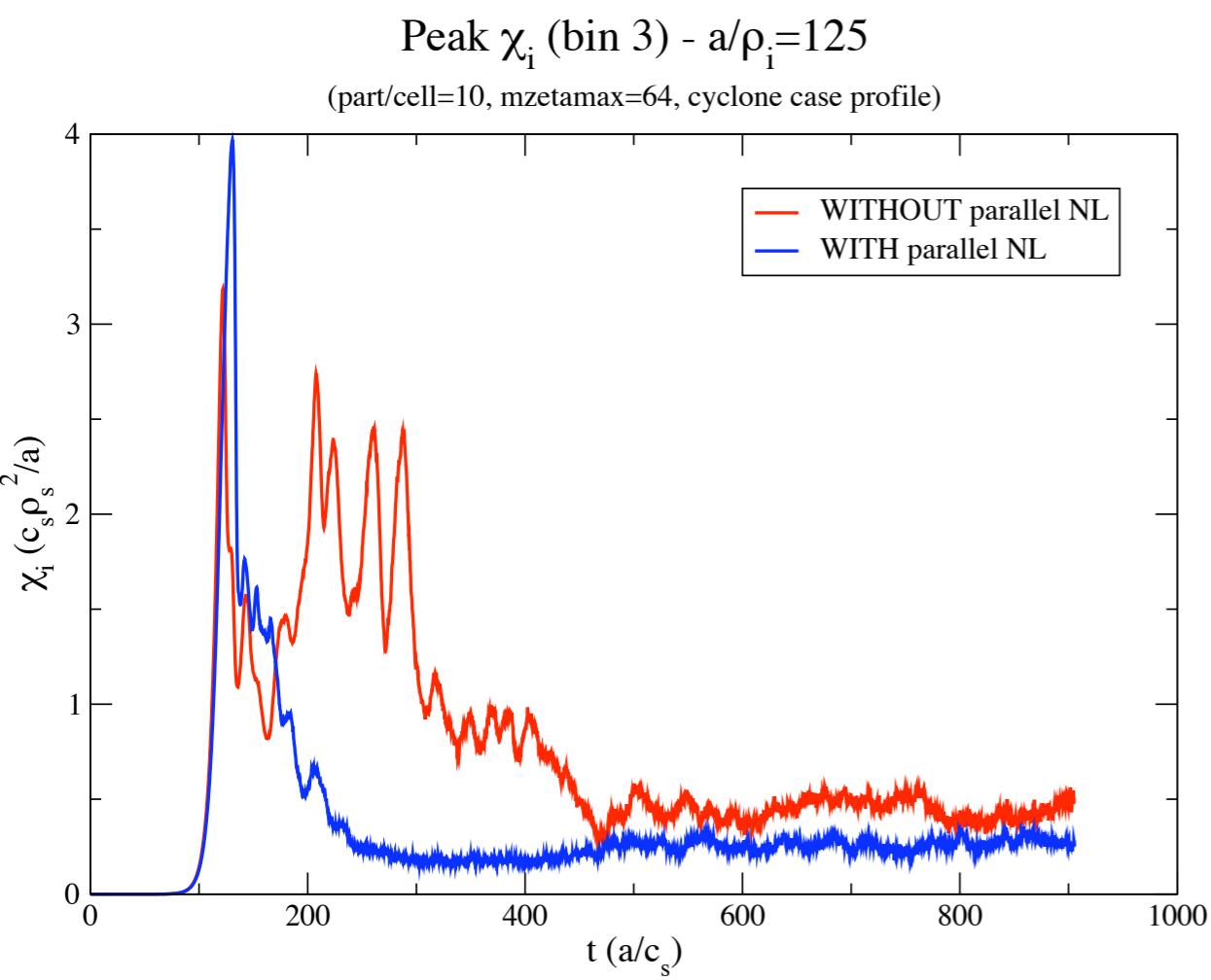
GTC - Particle Code

GYRO - Continuum Code

PG3EQ - Particle Code







Entropy Production - ITG modes

- δf -formulation: $F_i = F_{0i} + \delta f_i$, ν is the collision frequency, and Q_{ix} is the radial ion energy flux

$$\frac{\partial}{\partial t} \left\langle \int \frac{\delta f_i^2}{F_{0i}} dv_{\parallel} + \tau \phi^2 + \tau |\nabla_{\perp} \phi|^2 \right\rangle + \left\langle \tau \frac{\partial \phi}{\partial x_{\parallel}} \int v_{\parallel} \frac{\delta f_i^2}{F_{0i}} dv_{\parallel} + 2\tau \nu \int \frac{dv_{\parallel}}{F_{0i}} \left(\frac{\partial \delta f_i}{\partial (v_{\parallel}/v_{ti})} + \frac{v_{\parallel}}{v_{ti}} \delta f_i \right)^2 \right\rangle = \kappa_{Ti} \langle Q_{ix} \rangle$$

$$\tau \equiv T_e/T_i, \quad \kappa_{Ti} \equiv -d \ln T_{0i} / dx, \quad \langle \dots \rangle \equiv \frac{1}{V} \int d\mathbf{x},$$

- Let $w \equiv \delta f_i/F_{0i}$, $E_{\parallel} \equiv -\partial \phi / \partial x_{\parallel}$, $\partial \delta f_i / \partial (v_{\parallel}/v_{ti}) \approx -\beta \delta f_i$, $\beta \ll 1$, N is the particle number,

$$\frac{\partial}{\partial t} \sum_{j=1}^N \frac{w_j^2}{1-w_j} + \tau \frac{\partial}{\partial t} \langle \phi^2 + |\nabla_{\perp} \phi|^2 \rangle + \sum_{j=1}^N \left[-\tau E_{\parallel j} v_{\parallel j} + 2\nu\tau(1-\beta)^2 \left(\frac{v_{\parallel j}}{v_{ti}} \right)^2 \right] \frac{w_j^2}{1-w_j} = \kappa_{Ti} \langle Q_{ix} \rangle$$

- Energy balance:

$$\sum_{j=1}^N E_{\parallel j} v_{\parallel j} w_j = \frac{1}{2} \frac{\partial}{\partial t} \sum_{j=1}^N v_{\parallel j}^2 w_j \approx \frac{1}{2} \frac{\partial}{\partial t} \sum_{j=1}^N \alpha v_{ti}^2 w_j, \quad \alpha \approx 1 \quad or \quad \alpha \ll 1$$

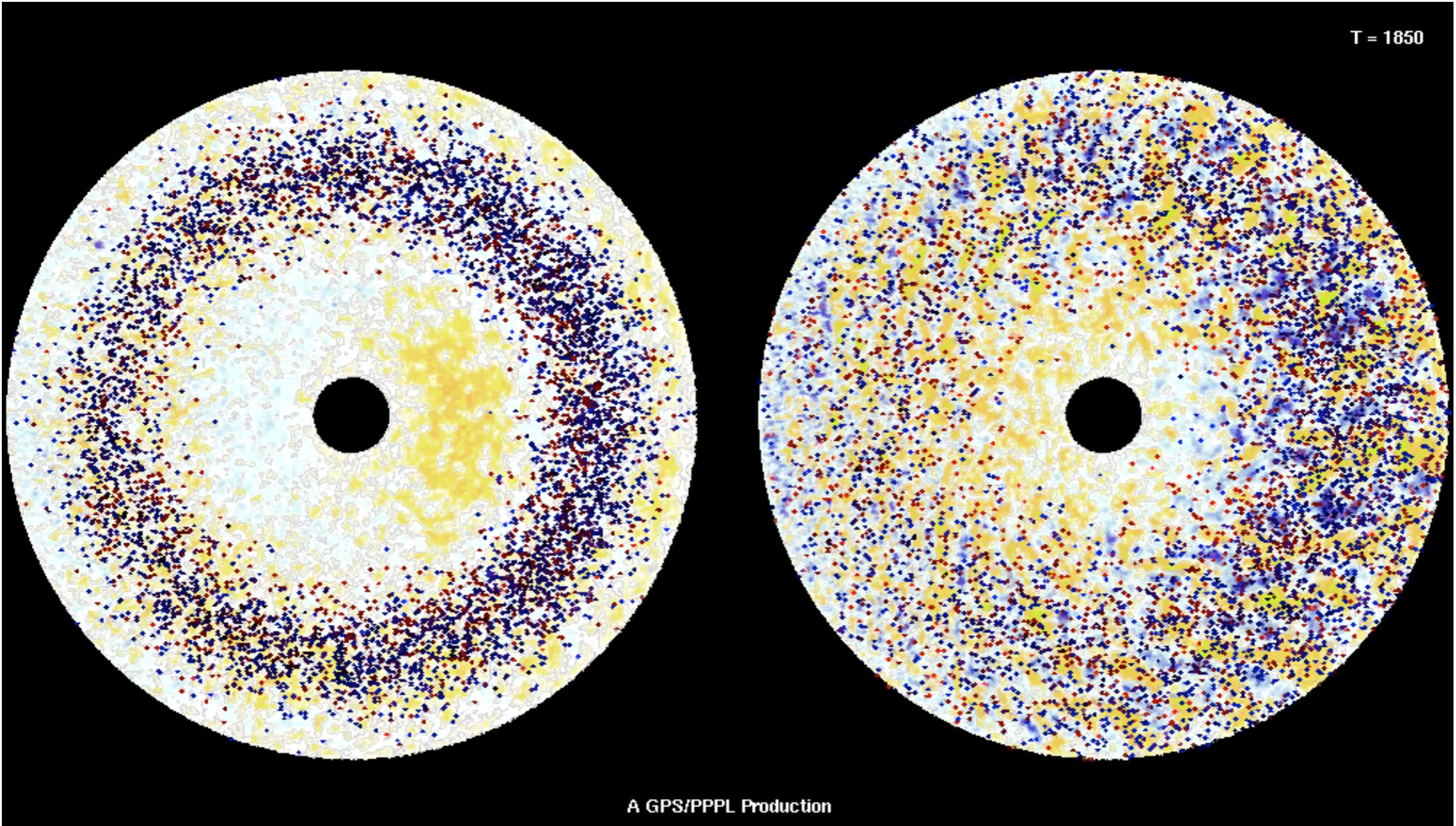
- In the steady state ($\partial/\partial t \langle \phi^2 + |\nabla \phi|^2 \rangle = 0$), with $w \ll 1$:

$$\frac{\partial}{\partial t} \sum_{j=1}^N \left(1 - \frac{\alpha}{4} \right) w_j^2 + 2\nu\tau(1-\beta^2)\alpha \sum_{j=1}^N w_j^2 = \kappa_{Ti} \langle Q_{ix} \rangle$$

Velocity-Space nonlinearity reduces ion energy flux, but collisions enhance it.

Particle Diffusion due to Toroidal ITG Modes

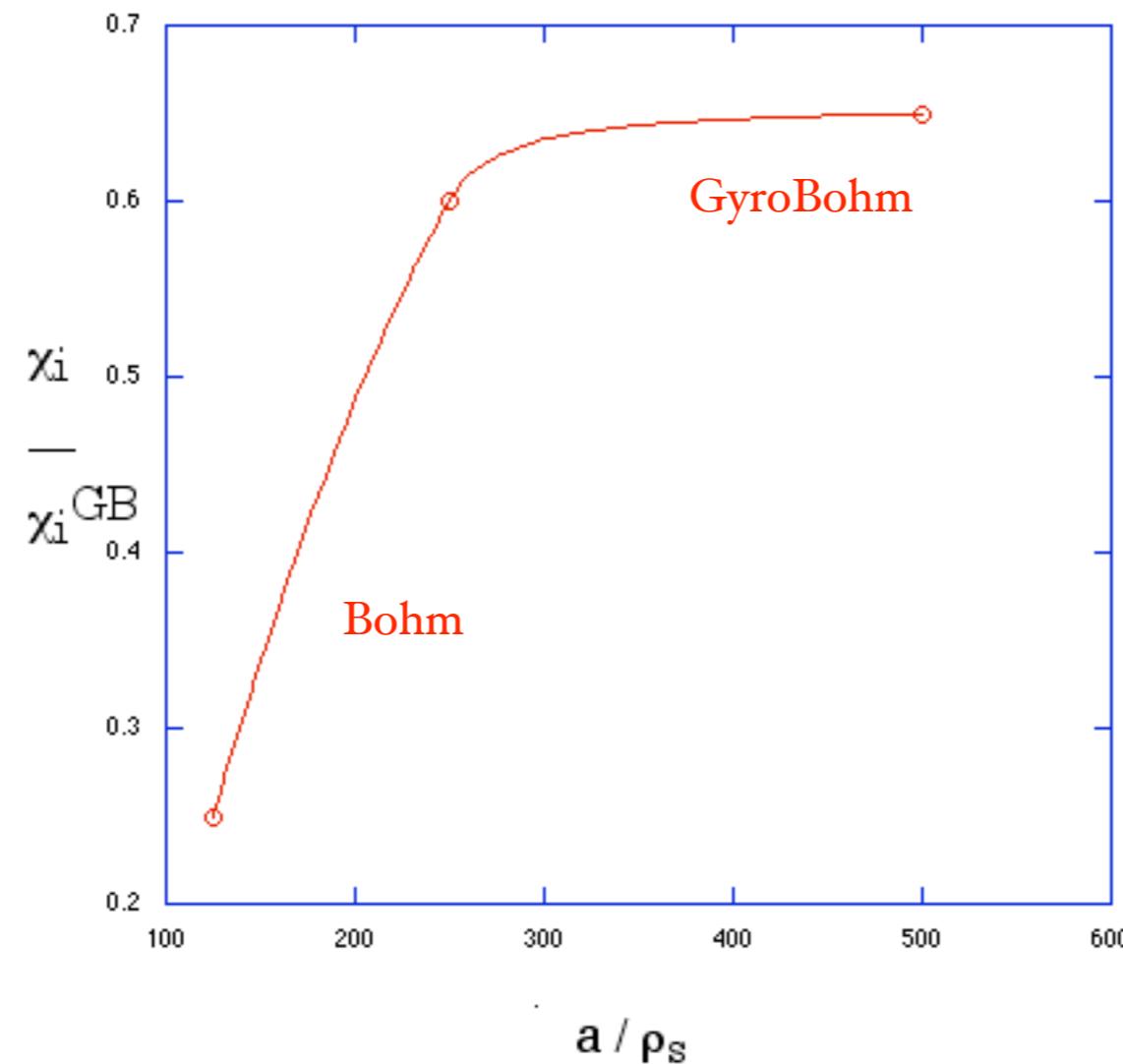
19



With
Parallel Velocity-Space Nonlinearity
GyroBohm?
Without
Bohm?

Data Management and Visualization
[Klasky, Ethier in collaboration with Beck, Ma]

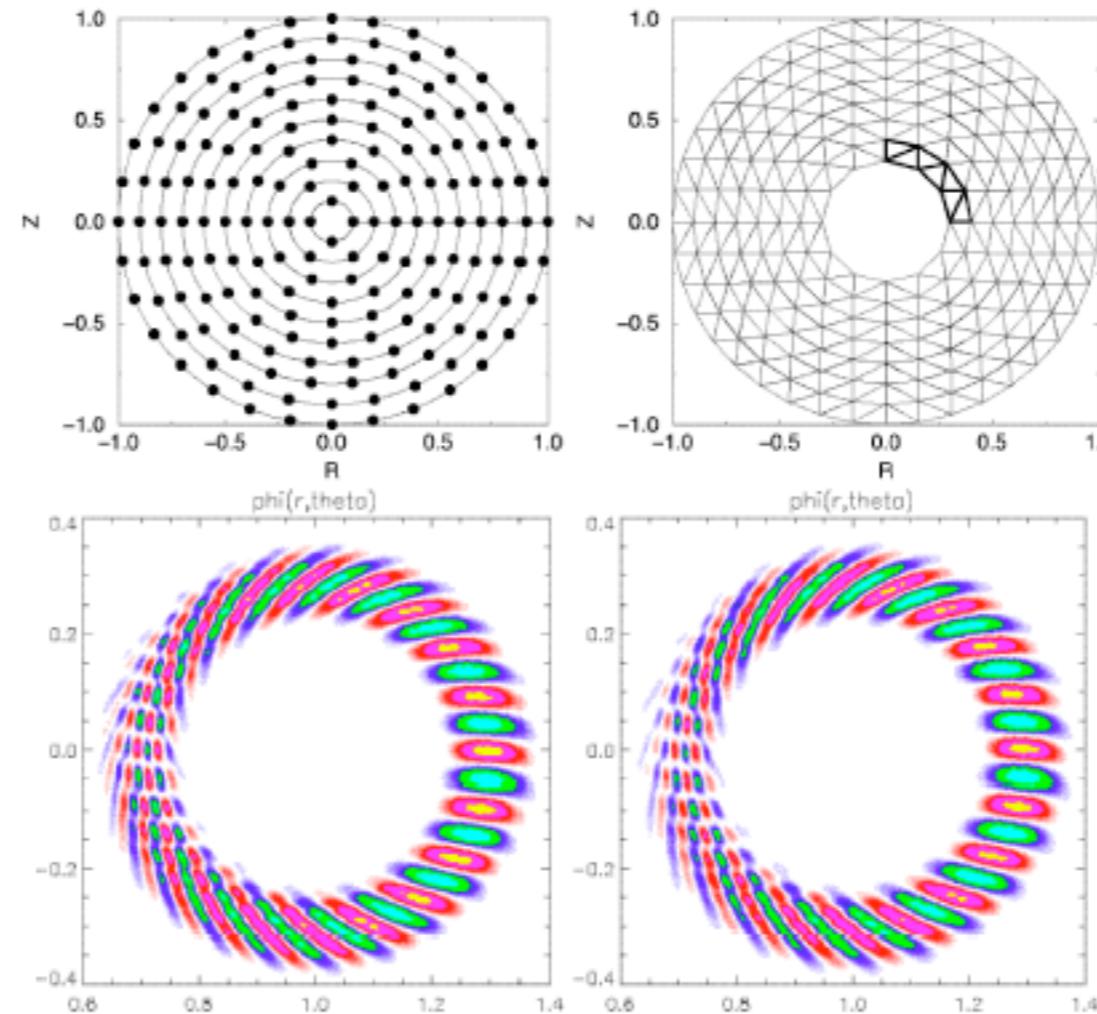
Transition from Bohm to GyroBohm similar to Lin, Ethier, Hahm and Tang, PRL '02?



Code Development - Finite Element Poisson Solver via PETSc

Old GTC solver vs. New GTC solver

[Nishimura et al., submitted to JCP]

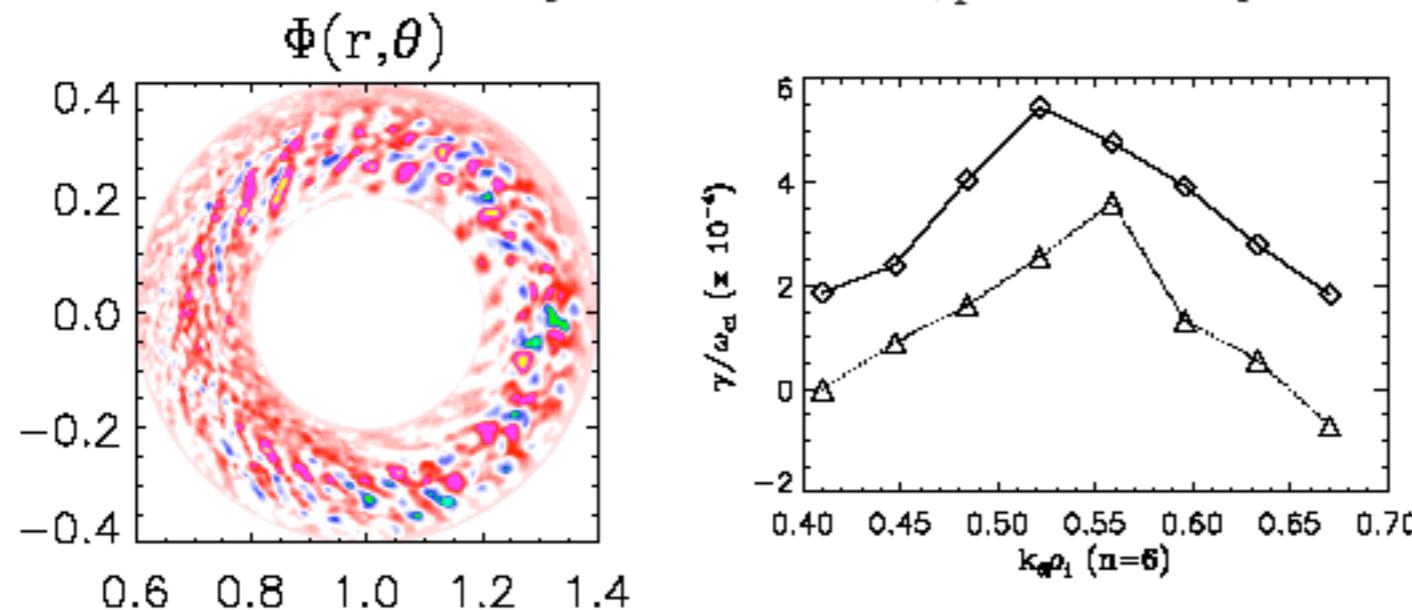


Collaboration with SciDAC-TOPS: D. E. Keyes and M. Adams

Split-weight Scheme for Toroidal Plasmas

PPPL

[J.L.V. Lewandowski, poster EP1.054]

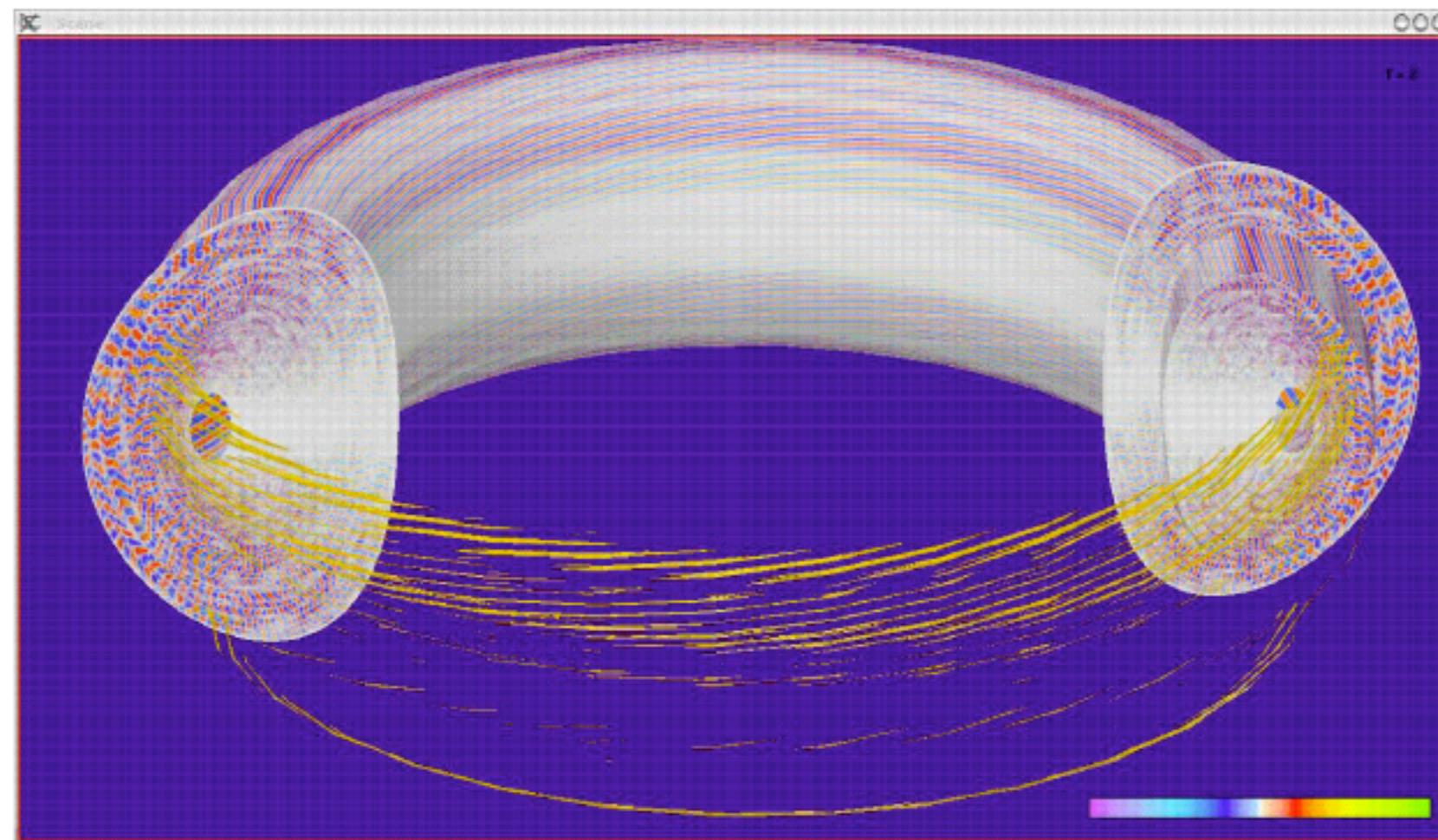


Parameters: $R_0/L_n = 2.22$, $R_0/L_{T_i} = R_0/L_{T_e} = 6.92$, $r/a = 0.5$.

- Split-weight scheme resolves non-adiabatic electron response only (allows for turbulent & collisional friction between trapped and untrapped electrons)
- Extension from sheared-slab 1D to toroidal geometry completed.
- Global finite element Poisson solver used to invert $L \partial_t \Phi = S$ (32 to 64 different stiffness matrices L)
- Numerical method is stable for large time step $\Delta t = 5 - 10 \omega_{ci}^{-1}$

Code Development - Shaped Plasmas

[Wang, Klasky and Ethier]



Core-Edge Simulations via GTC

- Basic requirements for the validity of gyrokinetic Vlasov-Maxwell equations are:

$$\rho/L_B \sim o(\epsilon),$$

$$\partial F/\partial\phi = 0,$$

$$d\mu_B/dt = 0.$$

- GTC already has Lorentz collision operators for e-i, and momentum and energy conserving collision operators for like species.

- The core uses the δf scheme of

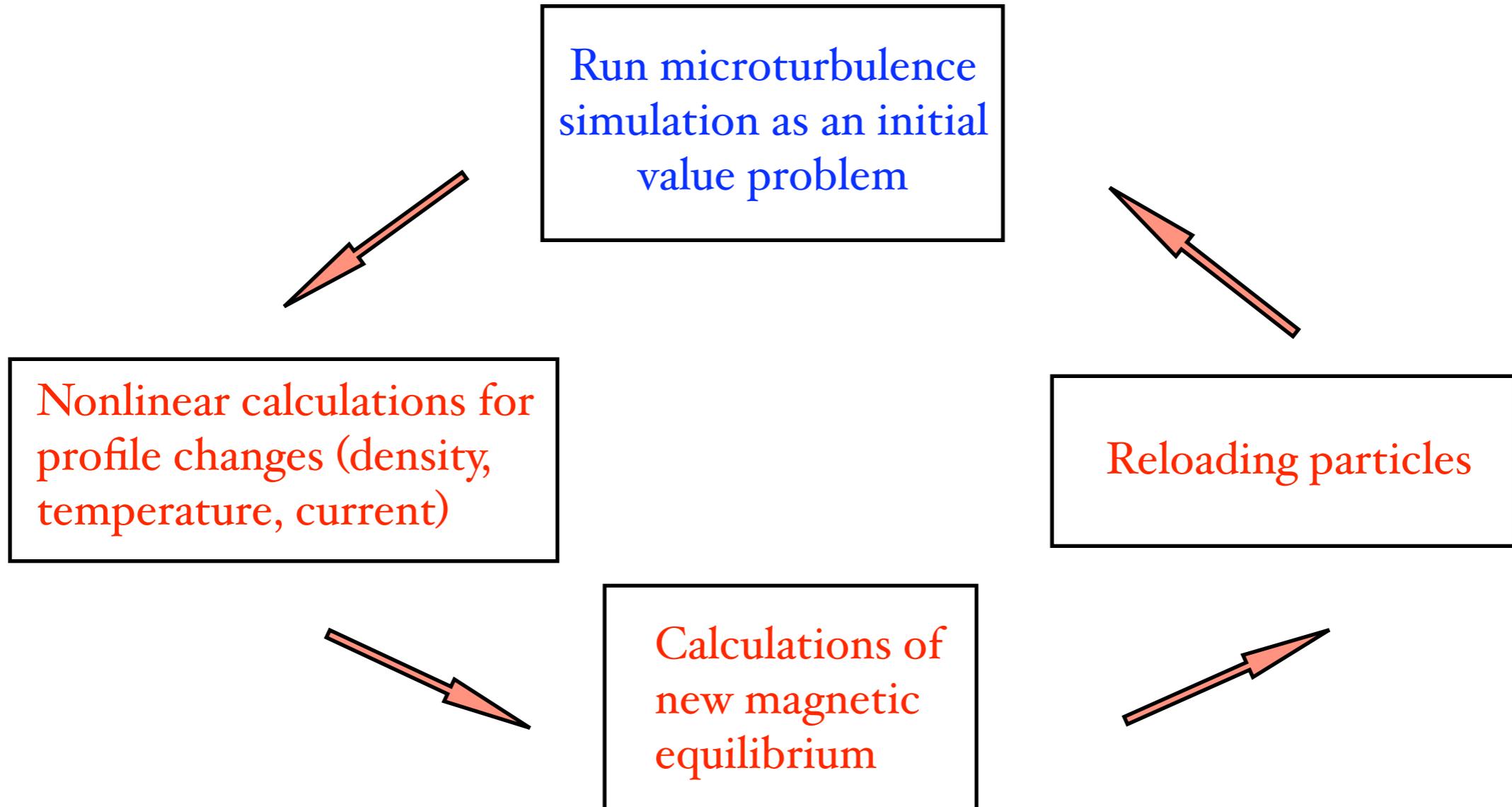
$$\frac{D\delta f}{DT} = -\frac{DF_0}{Dt}.$$

- The edge uses the δf scheme of

$$\delta f = F - F_0.$$

- Core-edge simulation inside the separatrix using GTC with electrons and multi-species ions is feasible.

Turbulence Simulation in Transport Time Scale



Conclusions

- Gyrokinetic Particle Simulation is a vital tool for fusion research
- Gyrokinetic formalism is most suitable for tokamak and stellarator physics when FLR effects, inertial effects and linear and nonlinear wave-particle interactions are important
- Gyrokinetic PIC toroidal simulation is an international effort:
GTC, GEM, PG₃EQ, GT₃D (JAERI), ORB₅(CRPP)
- Team coding: version control, developer's manual, OO (with V. Decyk)
- Strong candidate for Integrated Fusion Simulation Project

Related GTC papers:

- J. Lewandowski et al.-- Kinetic electrons using split-weight scheme [EP_I.054]
Y. Nishimura et al. -- Alfvén physics using hybrid scheme [CP_I.048]
W. X. Wang et al. -- Global simulation of shaped plasmas [CP_I.047]
Z. Lin et al., -- Global ETG modes [NI_I.003]
S. Ethier et al.-- GTC performance on MPP platforms [HP_I.014]
T. S. Hahm et al., -- Turbulence Spreading [EP_I.063]
T. G. Jenkins et al. -- Parallel velocity space nonlinearity in slab [CP_I.053]